1-Octadecanol 112-92-5 | DTXSID8026935

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Marada I	D. L.
Model	Data
110001	Bata

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 1.86e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.60e-01

Confidence level: 5.69e-01

Nearest Neighbors from the Training Set

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1-Bromooctadecane Measured: 2.70e-06 Predicted: 8.30e-06

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Heneicosane Measured: 4.52e-08 Predicted: 1.71e-05

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1-Hexadecene Measured: 3.85e-05 Predicted: 1.74e-03

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Undecane, 1-fluoro-Measured: 6.23e-08 Predicted: 2.52e-01